NSF Highlights

Thermodynamics Indicate Iron Oxide Clusters' Reactions with Molecular Precursors are Favorable

Outcome/Accomplishments

Experimental evidence shows that iron oxide clusters (Figure 1) play a critical role in the formation of hazardous compounds including persistent free radicals, dioxins and furans. Computational methods have identified the structures and thermodynamics of the initial steps in the reaction of iron oxide clusters and free radical precursors (Figure 2). Combined with experimental validation, this work helps to understand and mitigate the production of toxic materials.

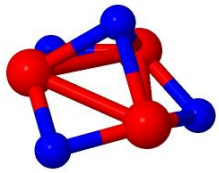

Figure 1. Fe_3O_4 cluster. Credit: Randall Hall, Louisiana State University

Impact/Benefits

Persistent free radicals, dioxins, and furans are formed during combustion processes such as cigarette smoking and auto exhaust. Determining the formation mechanism for these compounds is critical to prevent pollution formation. The toxicity of these materials have been categorized by the EPA as Class I, the most toxic class.

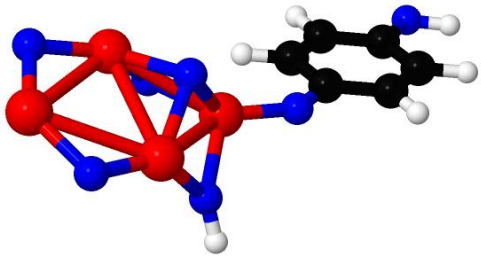

Figure 2. Reaction product of hydroxylated Fe_4O_5 with phenol. Credit: Randall Hall, Louisiana State University

Background

The adsorption of dioxin and furan precursors to the surface of metal oxide nanoparticles has been implicated as a crucial first step in the formation of dioxins and furans. Environmentally persistent free radicals are formed on these small particles, which can be inhaled deep into human lungs and cause cardiopulmonary disease. These initial steps can be quantified experimentally (Figure 2) and modeled with computational methods (Figure 1). Computational studies, when combined with experimental verification, offer the possibility of identifying the reaction site on the nanoparticles. Both dioxin and free radical formation can be better understood so that their formation and human exposure can be minimized.